

Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)

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Mission Statement: *To synthesize geomaterials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials.*

Successful operations of energy recovery and storage, sensor technologies, membranes for air and water purification, and catalytic processes require a fundamental understanding of the interactions of fluids at solid interfaces. There is considerable evidence that the known laws of adsorption, reaction, phase transitions, flow and mechanical strength are affected by the presence of fluids confined in porous geomaterials with nanometer-sized pores.

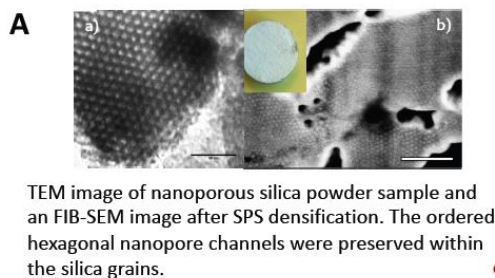
To accomplish transformational changes in energy science, MUSE will 1) develop a fundamental understanding of confinement and surface interactions in geomaterials on fluid phase behavior, reactivity, and multiphase flow properties; 2) examine the impact of mineralogy and material heterogeneity on chemo-mechanical properties; 3) determine *in-operando* cross-scale structural and microstructural material properties with fluids in confinement; and 4) develop validated multiscale and multi-physics models of mechanics, phase behavior, and flow that capture the observed chemo-morphological coupling.

MUSE will be organized into four *Research Thrust Areas*: (1) Material Architecture and Characterization, (2) Property Measurements, (3) Dynamic Characterization, and (4) Multiscale Multiphysics Modeling. Novel geo-architected materials developed in Thrust 1 will be used as substrates for determining properties of multi-phase fluids in heterogeneous confined architectures in Thrust 2, and for dynamic *in-operando* determination of material and fluid properties in Thrust 3. These measurements will inform the development of *experimentally-validated, atomistically-informed* modeling tools and frameworks in Thrust 4.

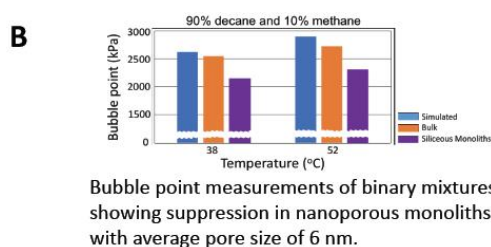
The project concept is shown in figure 1. Hierarchical nanostructured geomaterials with increasing levels of complexity will be created and characterized. (examples of this work from members of the team are shown in Figure 1A). Experiments with similarly-ordered, naturally occurring materials such as shales will also be performed. Phase behavior, flow and mechanical properties measurements will demonstrate chemo-mechanical interactions. The extent of bubble point suppression in siliceous nanoporous monoliths in experiments performed by members of the team is shown in Figure 1B. These new phase transition measurements in architected geomaterials at realistic conditions provide confirmation of modeling findings. In-operando observation of such phenomena will generate enhanced understanding of how confinement and surface interactions are affecting these properties.

The Dynamic Characterization focus area will develop *in situ (in-operando)* observation methods at system conditions. X-ray and neutron radiation provided by Basic Energy Sciences (BES) facilities allows the research team to probe the structure and dynamics of matter spanning from the molecular to the macro length scales (Figure 1C). Detailed nonreactive and reactive molecular dynamics (MD) modeling, enhanced by first principles quantum mechanics calculations, will be applied to improve fundamental understandings of, 1) phase behaviors of multicomponent fluids confined in nanometer size pores, 2) heterogeneous adsorption of fluid molecules on the heterogeneous surfaces of organic and inorganic materials, and 3) diffusion of fluid molecules within nanopores, and 4) reaction-induced mechanical deformations of nanostructures (Figure 1D).

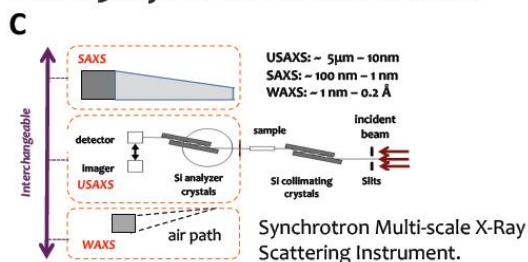
Thrust 1: Material Architecture & Characterization



Thrust 2: Measurement of Properties



Thrust 3: Dynamic Characterization



Thrust 4: Multiscale Modeling

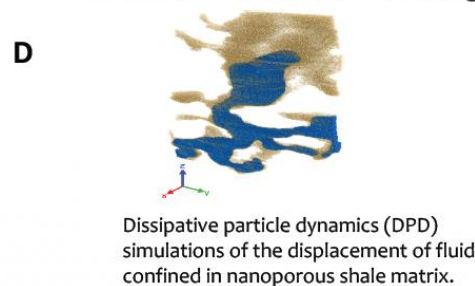


Figure 1: The four Thrust Areas of MUSE.

The Center will generate new data and create new models on phase transitions, flow characteristics, and multiphase properties in confined geomaterials. MUSE will bring together a multi-disciplinary team to establish a multi-scale scientific basis for advancing energy technologies that are of critical importance to the current and future world energy security and environmental sustainability.

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